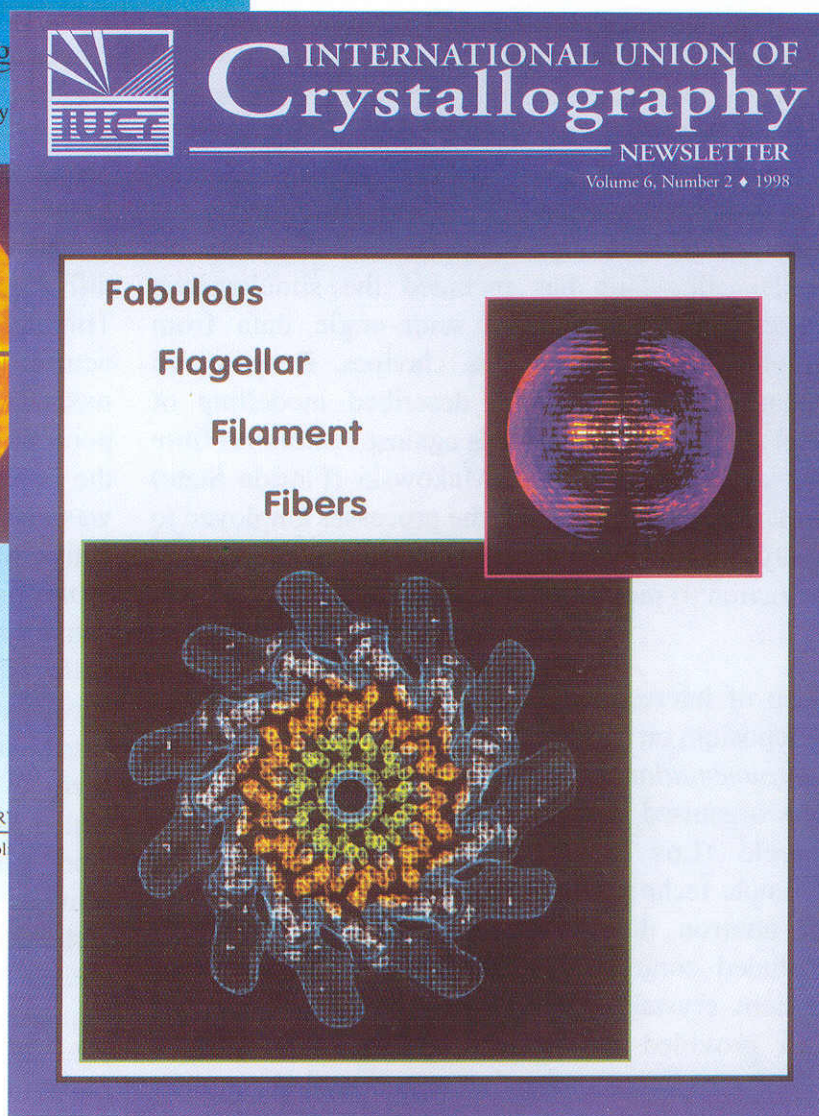
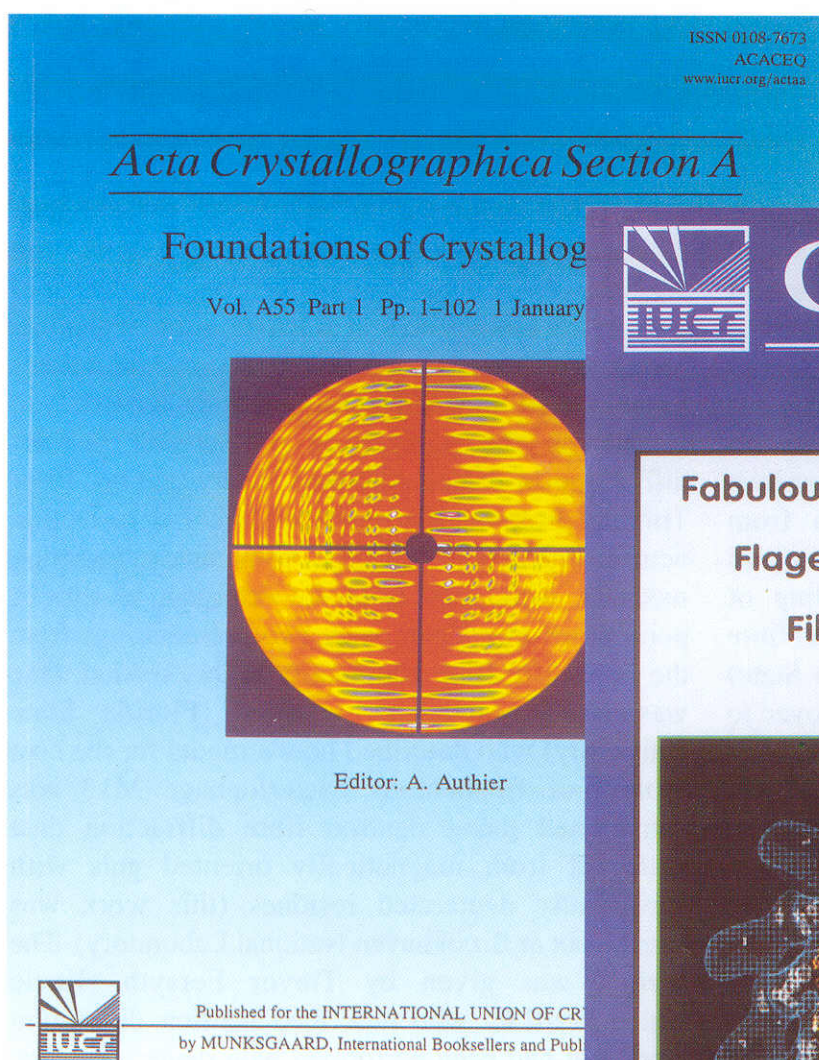


methods for calculating fibre diffraction patterns from polycrystalline fibres in which there are quite general and complicated forms of disorder. The

methods are used to analyse the disorder present in two polynucleotide fibres.

Rick Millane, Purdue University



## American Crystallographic Association Annual Meeting, Arlington, Virginia, 23<sup>rd</sup> July 1998

The Special Interest Group session, *The state of the art in fibre diffraction* was held on the final day of the ACA annual meeting in Arlington, Virginia. The session was organised and introduced by Gerald

Stubbs (Vanderbilt), who described the range of fibre diffraction experiments and current difficulties with weakly scattering samples, the short data collection times required for time-resolved experiments and the



need for improved resolution. He illustrated these problems with reference to his own work on tobamoviruses and other filamentous viruses. Tom Irving (IIT) described the facilities available at BioCAT at the Advanced Photon Source with careful use of TLA's (three-letter acronyms). Shyam Baskaran (Purdue) gave an account of progress in producing optimal Fourier difference maps from fibre diffraction data. Dan Kirschner (Boston) talked about the approaches he has employed to elucidate the folding and molecular organisation of amyloid proteins. A combination of magnetic alignment, small and wide-angle data collection and the use of known beta-pleated sheet atomic coordinates is proving fruitful in accounting for the observed polymorphism of amyloid. David Grubb (Cornell) gave an entertaining description of his work on spider silk. This has included the simultaneous collection of small and wide-angle data from dragline silk from *Nephila clavipes*. Rengaswami Chandrasekaran (Purdue) described modelling of triple-stranded nucleic acids against continuous fibre diffraction data and Lee Makowski (Florida State) took the audience through the processes employed to study variants of M13 bacteriophage from data reduction to molecular modelling.

Also of interest for fibre diffraction users was the symposium on *New Directions in Neutron Scattering Instrumentation for Structural Biology*. The session was organised by Benno Schoenborn and Bob von Dreele (Los Alamos National Laboratory) to promote technical developments for the application of neutron diffraction in structural biology. It included contributions from instrument scientists, protein crystallographers, and fibre diffractionists and provided numerous examples of important aspects of macromolecular structure that are best tackled using neutron diffraction rather than X-ray diffraction methods. There is now considerable interest in the use of image plates in neutron diffraction experiments since they offer a cheaper alternative to gas detectors and can easily record over a large solid angle. Such detectors have huge potential both in crystallography and in neutron fibre diffraction. Experiments that have been carried out on the new LADI diffractometer at the Institut Laue Langevin (ILL) on the location of solvent and hydrogen positions in lysozyme (Nimura, JAERI), concanavalin A (Helliwell, Manchester) and cob(II)alamin (Langan, LANL) have demonstrated the scope of image plate technology in neutron

diffraction. Although the main limitation for this technology remains the sensitivity of the plates to gamma radiation, the ongoing development of new phosphors with low gamma sensitivity is likely to be extremely important in the future. The progress that has been made in this area to date was reflected in some extremely interesting presentations. Nobuo Nimura (JAERI) gave an exciting talk on the development of neutron image plate technology, both on LADI at the ILL and on BIX1 and BIX 2 at JAERI in Japan. John Helliwell (Manchester University) described his recent work on concanavalin A. Paul Langan described the design of a structural biology station at LANL – this will allow both single crystal and fibre diffraction experiments to be carried out. After a presentation by Bob von Dreele on the application of neutron powder diffraction in protein structure determination, Peter Timmins from the ILL described how low resolution neutron diffraction, in parallel with contrast variation methods, were used to locate detergent in various porin structures. There were two presentations from the fibre diffraction community in this session. One was from Magdalena Ivanova (Florida State University) who described how a model for the coat protein of filamentous bacteriophage M13 was constructed using neutron fibre diffraction data collected from magnetically oriented gels with specifically deuterated residues (this work was carried out at Brookhaven National Laboratory). The second was given by Trevor Forsyth (Keele University/ILL) who described neutron diffraction work that had been performed with deuterated fibre samples of DNA. The experiments were carried out at the ILL on instrument D19. D19 currently operates with a thin “banana” detector that captures only a limited amount of the available data at a given time. However, the upgrade that is planned for D19 involves the replacement of this detector by an array of 9 area detectors. This will improve the efficiency of the instrument by a factor of 15-20 and will consequently have an enormous impact on the quality, throughput and scope of neutron fibre diffraction experiments.

Richard Denny (Daresbury Laboratory) and Trevor Forsyth (ILL/Keele).